Rainer Ernst GLASER
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CURRICULUM VITAE

PERSONAL DATA

Birth Date	June 18, 1957.
Family	Julia Chang, married August 22, 1996. Kayla Glaser, b. Oct. 7, 1997, Columbia, Missouri. James Glaser, b. Aug. 12, 2001, Columbia, Missouri.
Interests	Reading, Astronomy, Cognition, Travel, Badminton, Swimming.
Languages	Bilingual in English and German. Read French, some Spanish.
Honors	Fellow of the American Association for the Advancement of Science. Fellow of the Royal Society of Chemistry.

PROFESSIONAL INTERESTS & PROJECTS

Professional Interest	***From Electronic Structure Theory to New Concepts in Chemistry*** Theoretical, Organic, and Materials Chemistry. Chemistry Education.
Current Projects	1. Polar Order in Crystalline Organic Molecular Materials 2. DNA Base Deamination and Cross-Link Formation 3. Catalysis: Olefin Polymerization and Oscillating Chemical Reactions 4. Heteroarene Reduction: Hypoxia Selective Cancer Chemotherapeutics 5. Heterocumulenes: Biomimetic, Reversible CO_2 Sequestration 6. Astrochemistry: Nucleobase Synthesis in Interstellar Space 7. Science Communication: *Chemistry is in the News* and Scientific Writing 8. Cross-Disciplinary Science Education: Mathematics and Life Sciences

CURRENT POSITION & EMPLOYMENT HISTORY

2010ff	Visiting Professor, Institute of Chemistry, Chinese Academy of Sciences, Beijing.
2003-	Full Professor, Department of Chemistry, University of Missouri-Columbia.
1995-2003	Associate Professor, Department of Chemistry, Univ. of Missouri-Columbia.
1989-95	Assistant Professor, Department of Chemistry, Univ. of Missouri-Columbia.
1987-89	Postdoctoral Research Associate, Department of Chemistry, Yale University. Adviser: Professor Kenneth B. Wiberg.

EDUCATION

1984-87	Ph.D. Program, Department of Chemistry, University of California, Berkeley. Adviser: Professor Andrew Streitwieser, Jr. Chemistry Ph.D., 1987.
1983-84	Eberhard-Karls-Universität Tübingen, Germany. Chemistry Diplom, 1984.
1982-83	University of California, Berkeley, College of Chemistry and Lawrence Berkeley Laboratory (LBL), Mol. and Mat. Research Division. Adviser: Professor Andrew Streitwieser, Jr. Chemistry Masters of Science, 1983.
1977-82	Eberhard-Karls-Universität Tübingen, Germany. Chemistry Vordiplom, 1980. Physics Zwischenprüfung, 1979.
1976-77	Military Service, Deutsche Bundeswehr.
1967-76	Kepler-Gymnasium, Freudenstadt, Germany. Abitur with highest honors and Chemistry Prize, 1976.

SERVICE

2012-18	Board Member, *Reaction Mechanisms Conference*, ACS, Div. Org. Chem.
2012-	Editorial Board Member, *Crystal Structure Theory and Applications*
2011-	Editorial Board Member, *Journal of Thermodynamics and Catalysis*
2011-	Honorary Editorial Board Member, *Reports in Organic Chemistry*
2011-	Editorial Board Member, *Life*
2009-	Editorial Board Member, *Astrobiology*
2009-	Editorial Board Member, *The Icfai University Journal of Chemistry*
2008-11	MU Faculty Development Advisory Committee
2007-10	MU Honorary Degrees Committee.
2005-8	UM Research Computing Advisory Group (RCAG).
2003-6	MU College of Arts & Science, Promotion & Tenure Committee. Chair '04-'06.
2000-3	MU Academic Grievance Panel.
1999-2003	MU Faculty Advisory Council, Educational Technologies at MU.
1999-2002	MU Academic Assessment Committee.
1998-2002	Advisory Board, *Journal of Organic Chemistry*.
1996-9	MU Study Abroad Advisory Council.
1995-9	MU Task Force for Research Computing.
1992-	Boards of Review for 15 Funding Agencies (>160 reviews).
1987-	Boards of Review for >70 Journals (>810 reviews).

FUNDING SOURCES

National Institutes of Health (NIGMS), National Science Foundation (DUE, PRISM), Petroleum Research Fund of the American Chemical Society (G, AC, SE), The Camille & Henry Dreyfus Foundation, NATO Collaborative Research Grant, Japan Society for the Promotion of Science.

PROFESSIONAL ORGANIZATIONS

Gesellschaft Deutscher Chemiker, since 1980.

Liebig-Vereinigung für Organische Chemie, since 1995.

Wöhler-Vereinigung für Anorganische Chemie, since 1995.

American Chemical Society, since 1982.

University of Missouri ACS Local Section, 1995-7, Secretary-Treasurer.

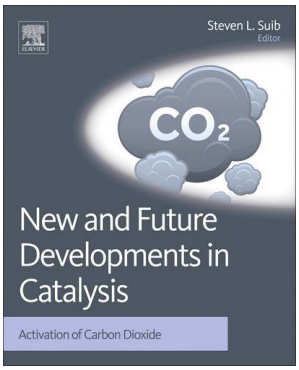
Div. of Org. Chem., since 1982. Div. Phys. Chem., since 1993. Theor. Chem. Subdivision, since 1993. Div. Chem. Toxicol., since 2001. Div. Chem. Educ., since 2001.

American Association for the Advancement of Science, since 1988. Elected Fellow 2004.

World Association of Theoretically Oriented Chemists, WATOC, since 1997.

A. Publications (160 published or accepted, 39 involved collaborations, Publication Spiegel, Citation Spiegel) | B. Patents (1) | C. Books (2)

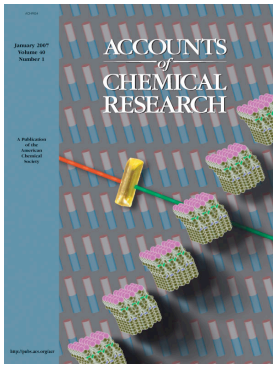
Items are numbered chronologically and listed in reverse chronological order. The online version (http://faculty.missouri.edu/~glaserr) contains direct links to online visualization materials and provides information on dissertations (22), invited conference presentations (52), departmental colloquia and seminars (120), contributed lectures (124), contributed poster, video & internet presentations (111), and media appearances (125).



Publ. 159, Aug. 2013.

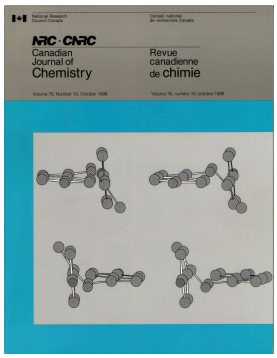
RMC2012, June 2012.

Ref. 144, May 2008.

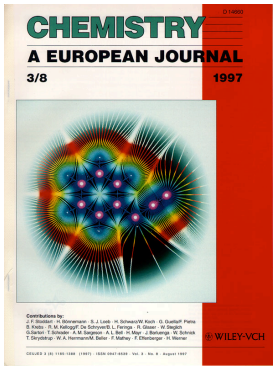


Publ. 140, Jan. 2007.

Ref. 137, July 2004.



Ref. 71, Oct. 1998.



Ref. 64, Aug. 1997.

A. Publications

160. Why the Acidity of Bromic Acid Really Matters for Kinetic Models of Belousov-Zhabotinsky Oscillating Chemical Reactions. Rainer Glaser, Marco Delarosa, and Ahmed Olasunkanmi Salau. *Invited Editorial*, *Journal of Thermodynamics and Catalysis* **2013**, *4*, in press.

159. Biomimetic Approaches to Reversible CO_2 Capture From Air. *N*-Methylcarbaminic Acid Formation in Rubisco-Inspired Models. Rainer Glaser, Paula O. Castello-Blindt, and Jian Yin. Chapter X in New and Future Developments in Catalysis. Activation of Carbon Dioxide, Steven L. Suib (Ed.), 1st ed. Elsevier Publishers: August **2013**.

158. Mechanistic Models for LAH Reductions of Acetonitrile and Malononitrile. Aggregation Effects

of Li^+ and AlH_3 on Imide-Enamide Equilibria. Rainer Glaser, Laura Ulmer, and Stephanie Coyle. *Article*, *Journal of Organic Chemistry* **2013**, *78*, 1113-1126. Publication Date (Web): Jan. 17, 2013. Publication Date (Print): Feb. 1, 2013.

157. 2,6-Dibenzhydryl-*N*-(2-phenyliminoacenaphthylenylidene)-4-chloroaniline nickel dihalides: Synthesis, characterization and ethylene polymerization for polyethylenes with high molecular weights. Shaoling Kong, Cun-Yue Guo, Wenhong Yang, Lin Wang, Wen-Hua Sun, Rainer Glaser. *Article*, *Journal of Organometallic Chemistry* **2013**, *725*, 37-45. Publication Date (Web): Dec. 2012. Publication Date (Print): Feb. 1, 2013.

156. Chloroyttrium 2-(1-(arylimino)alkyl)quinolin-8-olate Complexes: Synthesis, Characterization, and Catalysis of the Ring-Opening Polymerization (ROP) of ε-Caprolactone (ε-CL). Wenjuan Zhang, Shaofeng Liu, Wenhong Yang, Xiang Hao, Rainer Glaser and Wen-Hua Sun. *Article*, *Organometallics* **2012**, *31*, 8178-8188. Publication Date (Web): Nov. 5, 2012. Publication Date (Print): Dec. 10, 2012.

155. Disproportionation of Bromous Acid HOBrO by Direct O-Transfer and via Anhydrides $O(BrO)_2$ and $BrO\text{-}BrO_2$. An Ab Initio Study of the Mechanism of a Key Step of the Belousov-Zhabotinsky Oscillating Reaction. Rainer Glaser and Mary Jost. *Article*, *J. Phys. Chem. A* **2012**, *116*, 8352-8365. PDF. SI. Publication Date (Web): August 7, 2012. Publication Date (Print): August 16, 2012.

154. On the Reaction Mechanism of Tirapazamine Reduction Chemistry: Unimolecular N-H Homolysis, Step-Wise Dehydration or Triazene Ring-Opening. Jin Yin, Rainer Glaser, Kent S. Gates. *Article*, *Chem. Res. Toxicol.* **2012**, *25*, 634-645. PDF. SI. Publication Date (Web): March 5, 2012. Publication Date (Print): March 19, 2012.

153. Electron and Spin Density Analysis of Tirapazamine Reduction Chemistry. Jin Yin, Rainer Glaser, Kent S. Gates. *Article*, *Chem. Res. Toxicol.* **2012**, *25*, 620-633. PDF. SI. Publication Date (Web): March 5, 2012. Publication Date (Print): March 19, 2012.

152. Iodine Bonding Stabilizes Iodomethane in MIDAS Pesticide. Theoretical Study of Intermolecular Interactions between Iodomethane and Chloropicrin. Rainer Glaser and Kaitlan Prugger. *Article*, *J. Agric. Food Chem.* **2012**, *60*, 1776-1787. PDF. SI. Publication Date (Web): Feb. 8, 2012. Print Publication: Feb. 22, 2012.

151. Thermochemistry of the Initial Steps of Methylaluminoxane Formation. Aluminoxanes and Cycloaluminoxanes by Methane Elimination from Dimethylaluminum Hydroxide and Its Dimeric Aggregates. Rainer Glaser and Xinsen Sun. *Article*, *J. Am. Chem. Soc.* **2011**, *133*, 13323-13336. PDF. Publication Date (Web): August 5, 2011.

150. Asymmetric Imine *N*-Inversion in 3-Methyl-4-Pyrimidinimine. Molecular Dipole Analysis of Solvation Effects. Stephanie Coyle and Rainer Glaser. *Article*, *J. Org. Chem.* **2011**, *76*, 3987-3996. PDF. Publication Date (Web): April 18, 2011.

149. Asymmetry in the *N*-Inversion of Heteroarene Imines: Pyrimidin-4(3*H*)-Imine, Pyridin-2(1*H*)-Imine, and 1*H*-Purine-6(9*H*)-Imine. Rainer Glaser, Jian Yin, and Stephanie Miller. *Article*, *J. Org. Chem.* **2010**, *75*, 1132-1142. PDF. Publication Date (Web): January 28, 2010.1

148. Synthesis, Crystal Structure and Rotational Energy Profile of 3-Cyclopropyl-1,2,4-benzotriazine 1,4-di-N-oxide. Ujjal Sarkar, Rainer Glaser, Zack D. Parsons, Charles L. Barnes, and Kent S. Gates. *Article*, *J. Chem. Crystallography* **2010**, *40*, 624-629. PDF.

147. AMPAC 9. Semichem, 12456 W, 62nd Terrace, Suite D, Shawnee, KS 66216. www.semichem.com. Rainer Glaser. *Computer Software Review*, *J. Am. Chem. Soc.* **2009**, *131*, 13564. PDF.

146. *Chemistry Is in the News*: Assessing Intra-Group Peer Review. Kathleen M. Carson and Rainer E. Glaser. *Article*, *Assessment and Evaluation in Higher Education* **2009**, *34*, 69-81. (July 24, 2009). Link. PDF.

145. *Chemistry Is in the News*: The Why and Wherefore of Integrating Popular News Media into the Chemistry Classroom. Kathleen M. Carson, Deborah L. Hume, Yongqiang Sui, Susan Schelble, and Rainer E. Glaser. Chapter 16 in the *Chemists' Guide to Effective Teaching*, Vol. 2, Thomas J. Greenbowe, Melanie M. Cooper, and Norbert J. Pienta, Editors. Prentice Hall Series in Educational Innovation, Prentice Hall: Upper Saddle River, NJ, **2009**, 230-245. ISBN-13: 978-0-321-61195-6. ISBN-10: 0-321-61195-0. Available September 2008.

144. Cover of the May 29, 2008 Issue! Electronic Structures and Spin Topologies of γ-Picoliniumyl Radicals. A Study of the Homolysis of *N*-Methyl-γ-Picolinium and of Benzo-, Dibenzo-, and Naphthoannulated Analogs. Rainer Glaser, Yongqiang Sui, Ujjal Sarkar, and Kent Gates. *Article*, *J. Phys. Chem. A* **2008**, *112*, 4800-4814. PDF. DOI. (Online: May 22, 2008. In Print: May 29, 2008) Supporting Information.

143. *Ammonia Elimination from Protonated Nucleobases and Related Synthetic Substrates*. Ming Qian, Shuo Yang, Hong Wu, Papiya Majumdar, Nathan Leigh, and Rainer Glaser. *Article*, *J. Am. Soc. Mass Spectrometry (JAMAS)* **2007**, *18*, 2040-2057. PDF. Supporting Information.

142. *Adenine Synthesis in Interstellar Space: Mechanisms of Prebiotic Pyrimidine Ring-Formation in Monocyclic HCN-Pentamers.* Rainer Glaser, Brian Hodgen, Dean Farrelly, and Elliot McKee. *Article*, *Astrobiology* **2007**, *7*, 455-470. PDF. Online Visualization: Chime Displays and Reaction Animations.

141. *Stabilities and Spin Density Distributions of Benzannulated Benzyl Radicals.* Yongqiang Sui, Rainer Glaser, Ujjal Sarkar, and Kent Gates. *Article*, *J. Chem. Theory Comput.* **2007**, *3*, 1091-1099. PDF.

140. *Helically Annelated and Cross-Conjugated β-Oligothiophenes: An FT-Raman Spectroscopic and Quantum Chemical DFT Study.* Reyes Malavé Osuna, Rocío Ponce Ortiz, Victor Hernández, Juan Teodomiro López Navarrete, Makoto Miyasaka, Suchada Rajca, Andrzej Rajca, and Rainer Glaser, *Article*, *J. Phys. Chem. C* **2007**, *1*, 4854-4860. Online Visualization: Strong Raman Modes of beta-Oligothiophenes.

139. **COVER OF THE JANUARY ISSUE.** *Polar Order By Rational Design: Crystal Engineering With Parallel Beloamphiphile Monolayers.* Rainer Glaser. *Review*, *Acc. Chem. Res.* **2007**, *40*, 9-17.

138. *What's in a name? "Schall und Rauch"* versus *"Claim and Brand."* Rainer Glaser and Richard F. Murphy, *Letter*, *CrystEngComm*, **2006**, *8*, 948-951.

137. **COVER OF THE JULY ISSUE.** *Teaching Dissent and Persuasion.* Kathleen M. Carson, Brian Hodgen, and Rainer E. Glaser. *Review*, *Educ. Res. Rev.* **2006**, *1*, 115-120.

136. *Multifurcated halogen bonding involving Ph-Cl---H-CPh=N-R' interactions and its relation to idioteloamphiphile layer architecture.* Rainer Glaser, Richard F. Murphy, Yong-qiang Sui, Charles L. Barnes, and Sung Hoon Kim. *Communication*, *CrystEngComm* **2006**, *8*, 372-376.

135. *Perfect polar stacking of parallel beloamphiphile layers. Synthesis, structure, and solid-state optical properties of the unsymmetrical acetophenone azine DCA.* Rainer Glaser, Nathan Knotts, Ping Yu, Linghui Li, Meera Chandrasekhar, Christopher Martin, and Charles L. Barnes. *Invited Article*, *Dalton Trans.* **2006**, 2891-2899. Special issue: *Dalton Discussion 9: Functional Molecular Assemblies.*

134. *Embedding 1,6-Diphenyl-1,2-Dihydronaphthalene (DHN) in 1,4-Distyrylbenzene (DSB): Arene-Arene Interactions in a "Crossed Bis-Diarene."* Yongqiang Sui and Rainer Glaser. *Article*, *Cryst. Growth Des.* **2006**, *6*, 1014-1021. Online Visualization: Molecules, Pairs, Layers and Crystals.

133. *1-Methyl-1,3,6-triphenyl-7-(2-phenylpropenyl)-1,2-dihydronaphthalene*. Yongqiang Sui, Charles L. Barnes, and Rainer Glaser. *Communication*, *Acta Cryst. C* **2006**, *62*, 98-100.

132. *Dipole Parallel-Alignment in the Crystal Structure of a Polar Biphenyl: 4'-Acetyl-4-Meth-oxybiphenyl (AMB).* Rainer Glaser, Nathan Knotts, Zhengyu Wu, and Charles Barnes. *Article*, *Cryst. Growth Des.* **2006**, *6*, 235-240. Online Visualization: Molecular and Crystal Structures.

131. *Coordinate Covalent Ph-to-B Bonding in Phenylborates and Latent Formation of Phenyl Anions from Phenylboronic Acid.* Rainer Glaser and Nathan Knotts. *Article*, *J. Phys. Chem. A* **2005**, *109*, 1295-1304. Invited contribution to a Festschrift dedicated to Prof. William Hase on the occasion of his 60th birthday.

130. *Chemical Carcinogens in Non-Enzymatic Cytosine Deamination: 3-Isocyanatoacrylo-nitrile.* Rainer Glaser, Hong Wu, and Francisca von Saint Paul. *Article*, *J. Mol. Model.* **2005**, *11*, 731-737. Contribution to a Festschrift dedicated to Prof. Paul Schleyer on the occasion of his 75th birthday.

129. *Chemistry Is in the News. Assessment of Student Attitudes toward Authentic News Media Based Learning Activities.* Deborah L. Hume, Kathleen M. Carson, Brian Hodgen, and Rainer E. Glaser. *Article*, *J. Chem. Educ.* **2006**, *83*, 662-667.

128. *Oxanosine is a Substrate of Adenosine Deaminase. Implications for the Quest for a Toxico-logical Marker for Nitrosation Activity.* Papiya Majumdar, Hong Wu, Peter Tipton, and Rainer Glaser. *Article*, *Chem. Res. Toxicol.* **2005**, *18*, 1830-1841.

127. *Nitrosation Chemistry of Pyrroline, 2-Imidazoline, and 2-Oxazoline: Theoretical Curtin-Hammett Analysis of Retro-Ene and C-X Cleavage Reactions of alpha-Hydroxy-N-nitros-amines.* Hong Wu, Richard N. Loeppky, and Rainer Glaser. *Article*, *J. Org. Chem.* **2005**, *70*, 6790-6801.

126. *Nitrosative Cytosine Deamination. An Exploration of the Chemistry Emanating from De-amination with Pyrimidine Ring-Opening*. Sundeep Rayat, Ming Qian, and Rainer Glaser. *Article*, *Chem. Res. Toxicol.* **2005**, *18*, 1211-1218.

125. *Cytosine Catalysis of Nitrosative Guanine Deamination and Interstrand Cross-Link Formation.* Rainer Glaser, Hong Wu, and Michael Lewis. *Article*, *J. Am. Chem. Soc.* **2005**, *127*, 7346-7358.

124. *Additivity Schemes in Conformational Analysis. Concept and Demonstration.* Zhengyu Wu and Rainer Glaser. *Article*, *J. Theo. & Comput. Chem. (JTCC)* **2005**, *4*, 373-381.

123. *Amino-Effect on the Protonation of β-Aminoacrylonitrile*. Hong Wu and Rainer Glaser. *Communication*, *Chem. Res. Toxicol.* **2005**, *18*, 111-114.

122. *Demonstration of an Alternative Mechanism for G-to-G Cross-Link Formation.* Ming Qian and Rainer Glaser. *J. Am. Chem. Soc.* **2005**, *127*, 880-887.

121. *Chemistry Is in the News. Taxonomy of Authentic News Media Based Learning Activities.* Rainer E. Glaser and Kathleen M. Carson. *Int. J. Sci. Educ*. **2005**, *27*, 1083-1098.

120. *Structure of the Nitrosoguanidine Complexes of Nickel(II) and Copper(II) by X-ray Crystallography and Computational Analysis.* R. Kent Murmann, Rainer Glaser, and Charles Barnes. *J. Coord. Chem.* **2005**, *58*, 279-294.

119. *Structures of Nitro- and Nitrosoguanidine. X-ray Crystallography and Computational Analysis.* R. Kent Murmann, Rainer Glaser, and Charles Barnes. *J. Chem. Cryst.* **2005**, *35*, 321-329.

118. *Software for the Synergistic Integration of Science with ICT Education.* Zhengyu Wu and Rainer E. Glaser. *J. Inform. Tech. Educ. (JITE)* **2004**, *3*, 325-339.

117. *Nitrosative Guanine Deamination. Ab Initio Study of Deglycation of N-Protonated 5-Cyanoimino-4-Oxomethylene-4,5-Dihydroimidazoles*. Sundeep Rayat, Zhengyu Wu, and Rainer Glaser. *Chem. Res. Tox.* **2004**, *17*, 1157-1169. Visualization: Substrates, Products, Pre- & Post-Coordination Complexes, & Reaction Transition State Structures.

116. *5-Cyanoimino-4-oxomethylene-4,5-dihydroimidazole and 5-Cyanoamino-4-imidazolecarboxylic Acid Intermediates in Nitrosative Guanosine Deamination. Evidence from ^{18}O-Labeling Experiments.* Sundeep Rayat, Papiya Majumdar, Peter Tipton, and Rainer Glaser. *J. Am. Chem. Soc.* **2004**, *126*, 9960-9969.

115. *Ab Initio Study of the S_N1Ar and S_N2Ar Reactions of Benzenediazonium Ion with Water. On the Conception of "Unimolecular Dediazoniation" in Solvolysis Reactions.* Zhengyu Wu and Rainer Glaser. *J. Am. Chem. Soc.* **2004**, *126*, 10632-10639. Online Visualization: Molecular Structures and Transition Mode Animation.

114. *5-Cyanoimino-4-Oxomethylene-4,5-dihydroimidazole and Nitrosative Guanine Deamina-tion. A Theoretical Study of Geometries, Electronic Structures and N-Protonation.* Sundeep Rayat and Rainer Glaser. *J. Org. Chem.* **2003**, *68*, 9882-9892. Online Visualization: Structures.

113. *^{13}C-NMR Study of Halogen Bonding of Haloarenes. Measurement of Solvent Effects and Theoretical Analysis.* Rainer Glaser, Naijun Chen, Hong Wu, Nathan Knotts, and Martin Kaupp. *J. Am. Chem. Soc.*, *126*, 4412-4419. Online Visualization: Structures and Animations of Molecular Vibrations.

112. *Nitrosative Adenine Deamination: Facile Pyrimidine Ring-Opening in the Dediazoniation of Adeninediazonium Ion.* Brian Hodgen, Sundeep Rayat, and Rainer Glaser. *Communi-cation, Org. Lett.* **2003**, *5*, 4077-4080. Online Visualization: MP2 Structures.

111. *Polar Order in Crystalline Molecular Organic Materials by Rational Design*. Rainer Glaser, Nathan Knotts, and Hong Wu. *Review, Chemtracts* **2003**, *16*, 443-452.

110. *The Heterolytic Dissociation of Neutral and Protonated Nitrous Acid.* Hong Wu and Rainer Glaser. *J. Phys. Chem. A* **2003**, *107*, 11112-11119.

109. *5-Cyanoamino-4-Imidazolecarboxamide and Nitrosative Guanine Deamination: Experimental Evidence for Pyrimidine Ring-Opening During Deamination.* Ming Qian and Rainer Glaser. *Communication*, *J. Am. Chem. Soc.* **2004**, *126*, 2274-2275.

108. *Science Communication For All.* Rainer Glaser, *Feature*, *Chem. Internatl.* **2003**, *25*, 3-6.

107. *Ab Initio and Crystal Structures of (E,E)-1,4-Diphenylbuta-diene: A New Type of Arene-Arene Double T-Contact and an Interesting Inter-Layer Cooperation Involving Diastereoisomeric Contacts* . Rainer Glaser, Laxma R. Dendi, Nathan Knotts, Charles L. Barnes. *Cryst Growth Des.* **2003**, *3*, 291-300. Online Visualization: Ab Initio and Crystal Struc-tures of 1,4-Diphenylbutadiene.

106. *Synergism of Catalysis and Reaction Center Rehybridization. A Novel Mode of Catalysis in the Hydrolysis of Carbon Dioxide.* Michael Lewis and Rainer Glaser. *J. Phys. Chem. A* **2003**, *107*, 6814-6818.

105. *The Azine Bridge as a Conjugation Stopper: An NMR Spectroscopic Study of Electron Delocalization in Acetophenone Azines.* Michael Lewis and Rainer Glaser. *J. Org. Chem.* **2002**, *67*, 1441-1447. *Addition/Correction, J. Org. Chem.* **2002**, *67*, 7168.

104. *Theoretical Study of the Quadrupolarity of Carbodiimide.* Rainer Glaser, Michael Lewis, and Zhengyu Wu. *J. Phys. Chem. A* **2002**, *106*, 7950-7957.

103. *Synergism of Catalysis and Reaction Center Rehybridization in Nucleophilic Additions to Cumulenes: The One-, Two- and Three-Water Hydrolyses of Carbodiimide and Methyleneimine.* Michael Lewis and Rainer Glaser. *Chem. Eur. J.* **2002**, *8*, 1934-1944. Online Visualization: Reaction Paths of Three-Water Hydrolysis of Carbodiimide.

102. *Arene-Arene Double T-Contacts. Lateral Synthons in the Engineering of Highly Anisotro-pic Organic Crystals.* Michael Lewis, Zhengyu Wu, and Rainer Glaser. Chapter 7 in *Anisotropic Organic Materials - Approaches to Polar Order.* Rainer Glaser and Piotr Kaszynski, Editors. ACS Symp. Ser., Vol. 798, Am. Chem. Soc.: Washington, D.C., **2001**, p. 97-111.

101. *Nonlinear dye research leads to patent*. Rainer Glaser. *Newspaper Article*, *The Missourian*, Columbia, Missouri, February 15, **2001**.

100. *Aspirin. An Ab Initio Quantum-Mechanical Study of Conformational Preferences and of Neighboring Group Interactions.* Rainer Glaser. *J. Org. Chem.* **2001**, *66*, 771-779. Online Visualization: Structures of Aspirin, Benzoic Acid and Phenyl Acetate.

99. *Lattice Sum Calculations for 1/rp Interactions via Multipole Expansions and Euler Summations.* Don Steiger and Rainer Glaser. *J. Comp. Chem.* **2001**, *22*, 208-215.

98. *Tuning Intermolecular Interactions: A Study of the Structural and Vibrational Properties of p-Hexaphenyl under Pressure.* S. Guha, W. Graupner, R. Resel, M. Chandrasekhar, H. R. Chandrasekhar, R. Glaser, and G. Leising. *J. Phys. Chem. A* **2001**, *105*, 6203-6211.

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Published Version: http://www.prenhall.com/bruice
Local Version: http://www.missouri.edu/~chemrg/bruice3e

95. *Near-Perfect Dipole Parallel-Alignment in the Highly Anisotropic Crystal Structure of 4-Iodoacetophenone-(4-methoxyphenylethylidene) Hydrazone.* Michael Lewis, Charles Barnes, and Rainer Glaser. *Communication, J. Chem. Crystallogr.* **2000**, *30*, 489-496.

94. *Polarizabilities of Carbon Dioxide and Carbodiimide. Assessment of Theoretical Model Dependencies on Dipole Polarizabilities and Dipole Polarizability Anisotropies.* Michael Lewis, Zhengyu Wu, and Rainer Glaser. *J. Phys. Chem. A* **2000**, *104*, 11355-11361.

93. *A Higher Level ab Initio Quantum-Mechanical Study of the Quadrupole Moment Tensor Components of Carbon Dioxide.* Rainer Glaser, Zhengyu Wu and Michael Lewis. *J. Mol. Struct.* **2000**, *556*, 131-141. Contribution to a special issue in honor of Prof. Norman Allinger.

92. *Conformational Effects On The Quadrupolarity of Azines. An ab Initio Quantum-Mechani-cal Study Of A Lateral Synthon.* Rainer Glaser, Michael Lewis and Zhengye Wu. *J. Mol. Model.* **2000**, *6*, 86-98. Online Visualization: Optimized Structures.

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B. Patents

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